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Free vibrations of single walled carbon peapods

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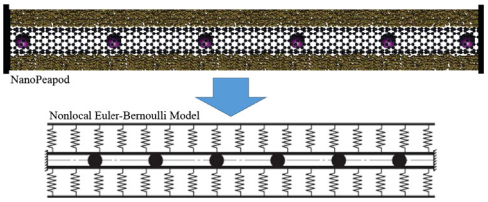
HIGHLIGHTS

- A nonlocal continuum model is developed for the lateral vibrations of nano-peapods resting on Winkler foundations.
- The small scale effects on the fundamental frequency is investigated and it is found that it may increase or decrease the fundamental frequency depending upon the foundation stiffness value.
- For any mass ratio there exist a certain foundation stiffness for which the fundamental frequency is independent of the small scale effect.

GRAPHICAL ABSTRACT



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ABSTRACT

In this paper the free vibration of single walled carbon nanopeapods encapsulating C_{60} molecules is considered. The nanopeapod is embedded in an elastic medium and clamped at both ends. The Euler–Bernoulli beam model is used for the carbon nanotube and the C_{60} molecules are considered as lumped masses attached to the beam. Based on the nonlocal elasticity theory the governing equation of motion is derived and the resonance frequencies of the nanopeapod are obtained. The effects of small scale, foundation stiffness and ratio of the fullerenes' mass to the nanotube's mass on the frequencies are studied and some conclusions are drawn.

1. Introduction

Research and progress in the field of carbon nanostructures developed after the discovery of C_{60} molecules in the mid 1980s. Discovery of carbon nanotubes in the early 1990s enhanced the research activities on the development of nanoscale electro mechanical devices. Since then, many studies have been performed to determine the structural, electrical, thermal and optical properties of nonotubes. Nanopeapods (NPPs) are carbon-nanotube-based hybrid structures which exhibit special physical properties with different potential applications. Carbon nanopeapods have very fascinating molecular, electronic and mechanical properties, distinct from those of the isolated components [1,2] which is the major motivation for the fabrication of novel molecular nanodevices [3]. The most common nanopeapod structure is the C_{60} fullerene nested at a single walled carbon nanotube (SWCNT) which is studied in detail by using a variety of experimental [1,4] and computational techniques [5–9].

The outstanding feature of nanotubes and nanopeapods as nanoscale electromechanical variable-frequency resonators, have attracted a lot of attention in the recent years. To provide a thorough understanding of how such nanostructures behave, one must acquire their mechanical and vibrational characteristics by

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experiments or theoretical simulations. Actually, experiments at nanoscale are expensive to operate. The perfect atomic simulations like Ab initio and molecular dynamics simulations are also computationally expensive for large systems [10,11]. Consequently, a great deal of research is focused on developing and using equivalent solutions such as continuum based modeling for the analysis of nanostructures to obtain acceptable results with less computational efforts. The bending and torsional buckling [12,13] and vibration characteristics [14] of nanotubes have been extensively addressed by many researchers using continuum models. Pradhan and Reddy [15] studied the buckling behavior of single walled carbon nanotube on Winkler foundation based on the Euler-Bernoulli beam theory. Rafiee et al. [16] investigated the geometrically nonlinear free and forced vibrations of simply supported SWCNTs. Kazemi-Lari et al. [17] analyzed the influence of viscoelastic foundation on the non-conservative instability of cantilever Carbon nanotubes (CNTs) based on a nonlocal Euler–Bernoulli beam model. Also the mechanical properties of NPPs have been predicted by continuum mechanics models in recent years. Sohi and Naghdabadi used a classic shell model to study the stability of C_{60} NPP under hydrostatic pressure [18] and also combined axial and radial pressure [19]. Asghari [20] utilized a nonlocal elastic shell model for NPPs to provide better predictions for the instability boundaries. Civalek and Demir [21] developed an elastic beam model for the bending analysis of microtubules based on the Euler–Bernoulli beam theory.

This study investigates the resonance frequencies of a bridged C_{60} carbon nanopeapod resting on a polymer foundation. To this aim an Euler–Bernoulli beam model based on the Eringen's nonlocal elasticity theory is utilized as the CNT's model and the buckyballs are considered as distributed point masses. Also the polymer foundation is simulated by the Winkler model. The variation of the resonances frequencies of the NPP versus the size effect parameter, foundation stiffness as well as the fullerenes' number and position are investigated.

2. Governing equations

Consider a carbon nanotube encapsulating buckyball molecules resting on a polymer matrix as shown in Fig. 1. The simplified model to be considered throughout the analysis is illustrated in Fig. 2 where the CNT and buckyballs are considered as an Euler–Bernoulli beam and point masses, respectively. Assuming an *xyz* frame where the *x*-axis coincides the CNT's axis, the elastic deformation field is described as

$$u_1(x,t) = u(x,t) - yw_{,x}(x,t) \tag{1}$$

$$u_2(x,t) = w(x,t) \tag{2}$$

$$u_3(x,t) = 0 \tag{3}$$

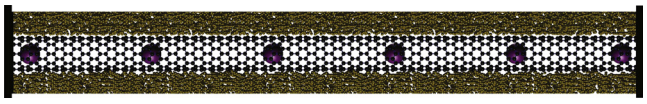

Fig. 1. Schematic view of a (10, 10) CNT, encapsulating some C_{60} molecules.

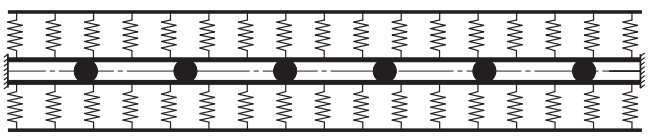

Fig. 2. Representation of the nanopeapod model by a beam resting on elastic foundation and distributed point masses.

where $u(x,t)$ and $w(x,t)$ are the longitudinal and transverse displacements, respectively and the comma subscript represents differentiation with respect to the following variable. Assuming an inextensible beam, the axial strain is

$$\varepsilon_{xx} = -yw_{,xx}(x,t) \tag{4}$$

and the other strain components are zero.

When the lattice spacing between the individual atoms of a nanostructure is considerable compared to the structural dimensions, using the continuum theory with the assumption of the continuity of the structure is essentially doubtful [22]. Namely, the classical continuum models will fail to simulate the structural behavior unless they are modified to include the size and nonlocal effects. The nonlocal elasticity theory of Eringen [23] proposes a modification to the classical elasticity theory which includes the small size features. Accordingly, the constitutive relation in one dimension for a linear elastic isotropic material is expressed as

$$\left(1-(e_0a)^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\sigma_{xx} = E\varepsilon_{xx} \tag{5}$$

where σ_{xx} is the normal stress and E is the elastic modulus. Also a is an internal characteristic length and e_0 is a material constant called the scaling effect to be determined from matching the experimental and lattice dynamics simulation data. For carbon nanotubes the characteristic length a is the length of the Carbon–Carbon bond, i.e. $a=0.142$ nm. Zhang and Sharma have shown [24] that the adopted value of the small-scale factor e_0 depends on the crystal structure in lattice dynamics and the nature of physics under investigation. They also estimated the scale coefficient $e_0 < 2$ nm for a SWCNT if the measured wave propagation frequency is greater than 10 THz.

Substituting Eq. (4) into Eq. (5), multiplying once by y and integrating over the cross-section yields the following relation in terms of the sectional bending moments (M_y):

$$M_y - e_0^2a^2M_{y,xx} = EIw_{,xx} \tag{6}$$

where EI is the bending stiffness of the CNT. From the principle of virtual work, the balance of forces and moments in the beam gives the equilibrium equation as follows:

$$M_{y,xx} + m\ddot{w} + kw = 0 \tag{7}$$

where m is the mass distribution along the NPP and k is the stiffness distribution of the foundation which is simulated by the Winkler model. Also the overdot represents differentiation with respect to time.

Applying the operator $\mathcal{L} = 1-(e_0a)^2\mathrm{d}^2/\mathrm{d}x^2$ to both sides of Eq. (7) and using Eq. (6), the governing equations of the NPP's transverse motion is obtained as

$$EIw_{,xxxx} + \mathcal{L}(mw_{,tt} + f_y) = 0 \tag{8}$$

where $f_y = kw$ is the force excreted by the elastic foundation on the NPP. Assuming the fullerene molecules as point masses nested at equal distance along the CNT of length l, the mass distribution over the NPP can be expressed as

$$m = m_0 + m_f\sum_{i=1}^{n}\delta(x-x_i) \tag{9}$$

where m_0 and m_f are the nanotube's mass per length and the fullerene's mass, respectively. The number of encapsulated fullerenes is represented by n and $x_i = iL/(n+1)$ represent the fullerenes' position by the Dirac delta function $\delta(x-x_i)$.

Assuming a pure harmonic vibration as

$$w(x,t) = \overline{w}(x)e^{i\omega_n t} \tag{10}$$

and using the Galerkin's technique, the solution to the governing equations can be expressed by the following modal expansion